SUPER-CORRELATION CONSISTENT COMPOSITE APPROACH (S-CCCA) FOR LATER 3D AND 4D TRANSITION METAL MOLECULES

BRADLEY WELCH, ANGELA K. WILSON, *Department of Chemistry, Michigan State University, East Lansing, MI, USA*.

The super-correlation consistent composite approach (s-ccCA) has been successful in the prediction of accurate dissociation energies for early 3d and 4d transition metal-containing species[a]. As one moves across the periodic table the computational cost requirements also increase. Thus, this increase in computational cost is an important consideration in the development of composite methodologies. Here we present s-ccCA for the late 3d and 4d transition metal molecules with an important modification, employing a simple Continued Fraction approximant. This approach was evaluated against s-ccCA results on the early 3d and 4d species. This reduced cost s-ccCA was then applied to the late 3d and 4d species, and the resulting dissociation energies were compared with state-of-the-art Resonant Two-Photon Ionization bond dissociation energies [bcd].

[a] Mol. Phys. 119, (2021)
[b] J. Chem. Phys. 153, 074303, (2020)
[c] J. Chem. Phys. 146, 144310, (2017)
[d] J. Chem. Phys. 151, 044302, (2019)